

Quantum Critical Points in Quantum Impurity Systems

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Abstract

The numerical renormalization group method is used to investigate zero temperature phase transitions in quantum impurity systems, in particular in the soft-gap Anderson model, where an impurity couples to a non-trivial fermionic bath. In this case, zero temperature phase transitions occur between two different phases whose fixed points can be built up of non-interacting single-particle states. However, the quantum critical point cannot be described by non-interacting fermionic or bosonic excitations.

Key words: Quantum Phase Transition, Soft-Gap Anderson Impurity Model, Numerical Renormalization Group

Impurity quantum phase transitions have recently attracted considerable interest (for a review see [1]). These transitions can be observed in systems where a zero-dimensional boundary (the impurity) interacts with a bath of free fermions or bosons. Examples include one or two magnetic impurities coupling to one or more fermionic baths [1] and the spin-boson model, where a two-level system couples to a bosonic bath [2,3]

A very well studied model is the soft-gap Anderson model [4]:

$$H = \varepsilon_f \sum_{\sigma} f_{\sigma}^{\dagger} f_{\sigma} + U f_{\uparrow}^{\dagger} f_{\uparrow} f_{\downarrow}^{\dagger} f_{\downarrow} + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + V \sum_{k\sigma} \left(f_{\sigma}^{\dagger} c_{k\sigma} + c_{k\sigma}^{\dagger} f_{\sigma} \right). \quad (1)$$

(Notations are standard.) This model has the same form as the single impurity Anderson model but for the soft-gap model we require that the hybridization function $\Delta(\omega) = \pi V^2 \sum_k \delta(\omega - \varepsilon_k)$ has a soft-gap at the Fermi level, $\Delta(\omega) = \Delta_0 |\omega|^r$, with an exponent $r > 0$.

The model eq. (1) shows a non-trivial zero-temperature quantum phase transition between a local moment phase (LM) and a strong coupling phase (SC) at a *finite* value of the coupling Δ_0 . Since the

first approach using a large degeneracy technique [4], intensive studies have been performed to clarify various properties of this model, such as the impurity susceptibility, specific heat and entropy [5,6], and dynamic quantities [7]. An important issue, which is far from being fully understood, is the characterization of the quantum critical points. To this end, we employ the numerical renormalization group method suitably extended to handle non-constant couplings $\Delta(\omega)$ [5,6]. This method allows a non-perturbative calculation of the many-particle spectrum and physical properties in the whole parameter regime of the model eq. (1), in particular in the low-temperature limit, so that the structure of the quantum critical points is accessible.

In Fig. 1, the many-particle spectra corresponding to the local moment (dotted lines), the strong coupling (dashed lines), and the quantum critical (QCP, lines with circles) fixed points of the symmetric soft-gap model are shown as functions of the exponent r (for a similar figure, see Fig. 13 in [5]). Each set of fixed points is extracted from the lowest six levels with quantum-numbers $Q = -1$, $S = 0$.

The fixed-point structure of the strong coupling and the local moment phase can be easily understood as that of a free conduction electron chain. The combination of the single-particle states of the free chain leads to the degeneracies seen in Fig. 3 below.

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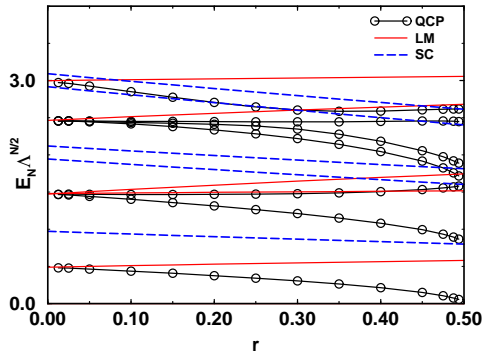


Fig. 1. Dependence of the many-particle spectra for the three fixed points of the symmetric soft-gap Anderson model on the exponent r .

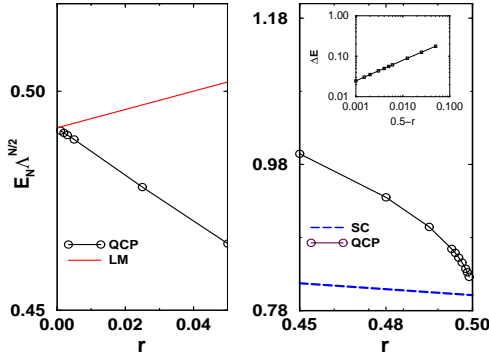


Fig. 2. Same data as in Fig. 1 for the region close to $r = 0$ (left panel) and $r = 0.5$ (right panel). The deviation between QCP and LM is linear for small r while the deviation between QCP and SC is proportional to $\sqrt{0.5 - r}$, as can be seen in the inset of the right panel.

What information can be extracted from such a level structure? First we observe that the levels of the QCP approach the levels of LM(SC) in the limits $r \rightarrow 0$ ($r \rightarrow 0.5$). The limiting behaviour is illustrated in Fig. 2: the QCP levels deviate linearly from the LM levels for $r \rightarrow 0$ while the deviation ΔE to the SC levels is proportional to $\sqrt{0.5 - r}$ for $r \rightarrow 0.5$. This has direct consequences for physical properties at the QCP; the local susceptibility at the QCP, for example, shows a square-root dependence on $(0.5 - r)$ close to $r = 0.5$ [5].

A plot similar to Fig. 1 can be calculated for the spin-boson model, using the numerical renormalization group method as in Ref. [3] (data not shown here). In the spin-boson model, the many-particle levels of the QCP turn out to approach the levels of the delocalized (localized) fixed point in the limit $s \rightarrow 0$ ($s \rightarrow 1$), with s the exponent of the bath spectral function $J(\omega) \propto \omega^s$.

It would be nice to compare these numerical results with a perturbative expansion around the limits $r = 0$ and $r = 0.5$. Such an expansion has been performed for small r in Ref. [8]. Interestingly, the linear deviation

between LM and QCP levels for small r cancels in the evaluation of the impurity contribution to the entropy, and the correction turns out to be $\propto r^3$. The level structure of the QCP itself might be accessible to perturbational approaches, at least in the limits $r = 0$ and $r = 0.5$; the deviations would then appear as marginal perturbations of the LM and SC fixed points.

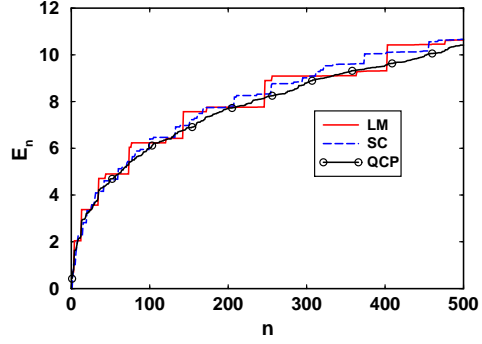


Fig. 3. Many-particle energies of the three fixed points of the symmetric soft-gap model versus the label n for $r = 0.3$.

An alternative way to characterize the spectra of the various fixed points is shown in Fig. 3 where we plot the many-particle energies E_n versus the label n which simply counts the many-particle states starting from the ground-state $n = 1$. Degeneracies due to symmetries of the model are not considered. We clearly see that the LM and SC fixed points show additional degeneracies as they are built up from single-particle excitations; this gives rise to the plateaus in E_n .

In the case of the quantum critical fixed points, degeneracies due to the combination of single-particle levels are missing, which indicates that the quantum critical point cannot be constructed from non-interacting single-particle states.

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